4-Hydroxy-3'-methoxybibenzyl

59586-27-5 | DTXSID40208245

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.05e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.07e-01

Confidence level: 6.61e-01

Nearest Neighbors from the Training Set

Image not found
Pentylparaben
Measured: 1.54e-04
Predicted: 1.40e-02

Image not found
N-Phenyldiethanolamine
Measured: 1.84e-01
Predicted: 4.75e-01

Image not found
Phenylpropanolamine
Measured: 1.32e-01
Predicted: N/A

Image not found
Naproxen
Measured: 6.91e-05
Predicted: 8.57e-03

Image not found
Butylparaben
Measured: 1.07e-03
Predicted: 5.24e-02